

Acetic acid  
64-19-7 | DTXSID5024394

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.33 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.13e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Formic acid</div> <div>Measured: 15.7</div> <div>Predicted: 51.1</div>	<div>Image not found</div> <div>Bromoacetic acid</div> <div>Measured: 3.53</div> <div>Predicted: 1.35e-01</div>	<div>Image not found</div> <div>Propionic acid</div> <div>Measured: 3.97</div> <div>Predicted: 3.47</div>
<div>Image not found</div> <div>Acrylamide</div> <div>Measured: 1.81</div> <div>Predicted: 1.36e-02</div>		